Renormalization group dependence of the QCD coupling

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The general relation between the standard expansion coefficients and the beta function for the QCD coupling is exactly derived in a mathematically strict way. It is accordingly found that an infinite number of logarithmic terms are lost in the standard expansion with a finite order, and these lost terms can be given in a closed form. Numerical calculations, by a new matching-invariant coupling with the corresponding beta function to four-loop level, show that the new expansion converges much faster.

It is of crucial importance to consider the renormalization group (RG) scale dependence of the strong coupling, in order to have full consistency in QCD and its applications [1, 2]. As is well known, the QCD running coupling $\alpha = \alpha_s/\pi = g^2/(4\pi^2)$ satisfies the RG equation

$$u\frac{\mathrm{d}\alpha}{\mathrm{d}u} = -\sum_{i=0}^{\infty}\beta_i\alpha^{i+2} \equiv \beta(\alpha), \qquad (1)$$

where the β function was calculated to one-loop level in QCD more than thirty years ago [3], to two-loop in Ref. [4], to three-loop in Ref. [5], and to four-loop in Ref. [6], in the minimal subtraction scheme [7]. It can be expressed as polynomials of the number of flavors N_{f}, i.e., $\beta_i(N_{\mathrm{f}}) = \sum_{j\geq 0}\beta_{i,j}N_{\mathrm{f}}^j$. The color factor $\beta_{i,j}$ is presently available to 4-loop level, i.e.,

$$[\beta_{i,j}] = \begin{bmatrix} 11/2 & -1/3 & 0 & 0 \\ 51/4 & -19/12 & 0 & 0 \\ \frac{2857}{64} & -\frac{5032}{576} & \frac{325}{1728} & 0 \\ \beta_{3,0} & \beta_{3,1} & \beta_{3,2} & \frac{1093}{93312} \end{bmatrix} \qquad (2)$$

with $\beta_{3,0} = 891\zeta_3/32 + 149753/768 \approx 228.4606573$, $\beta_{3,1} = -1627\zeta_3/864 - 1078361/20736 \approx -54.26788763$, $\beta_{3,2} = 809\zeta_3/1296 + 50065/20736 \approx 3.164758128$, where ζ is the Riemann zeta function, and $\zeta_2 = \pi^2/6$, $\zeta_3 \approx 1.202056903$, $\zeta_4 = \pi^4/90$, $\zeta_5 \approx 1.036927755$. In this paper, all color factors are given for $N_{\mathrm{c}} = 3$. Comparing the beta expressions here with those in Ref. [6], one would find a difference by a factor of 2^{2i+1}.

In practical applications, it is convenient to have an explicit expression of the α as a function of the renormalization point u. The standard approach is to expand it to a series of $L = 1/\ln(u^2/\Lambda^2)$, where Λ is the QCD scale parameter. However, how the expansion coefficients are connected to the beta function is not generally known, though one can find the relation to order 3 in Ref. [8], and to order 4 in Ref. [9]. In this letter, the general relation between the expansion coefficients and the beta

function are provided. It is accordingly found that an infinite number of terms like $\ln^j L$ are lost in the standard expansion with a finite order, and these lost terms can be given in a closed form. Numerical calculations, by a new matching-invariant coupling with the corresponding beta function to four-loop level, show that the new expansion, with the lost terms included, converges much faster.

To solve Eq. (1), let's define

$$\acute{\beta}(\alpha) \equiv \frac{\beta_0^2}{\beta_1}\left[\frac{1}{\beta(\alpha)} - \frac{\beta_1}{\beta_0^2\alpha} + \frac{1}{\beta_0\alpha^2}\right]. \qquad (3)$$

With the series expression for $\beta(\alpha)$ in Eq. (1), one can easily get an explicit expression

$$\acute{\beta}(\alpha) = \frac{\sum_{j=0}^{\infty}(\beta_0\beta_{j+2}/\beta_1 - \beta_{j+1})\alpha^j}{\sum_{i=0}^{\infty}\beta_i\alpha^i}, \qquad (4)$$

which indicates that $\acute{\beta}(\alpha)$ is analytic at $\alpha = 0$, and can thus be expanded to a Taylor series as

$$\acute{\beta}(\alpha) = \sum_{k=0}^{\infty}\acute{\beta}_k\alpha^k. \qquad (5)$$

The expansion coefficients $\acute{\beta}_k$ can be obtained from the normal mathematical formula

$$\acute{\beta}_k = \frac{1}{k!}\left.\frac{\mathrm{d}^k}{\mathrm{d}\alpha^k}\acute{\beta}(\alpha)\right|_{\alpha=0}. \qquad (6)$$

Another easy way to obtain these coefficients is to use the recursive relation

$$\acute{\beta}_k = \frac{\beta_{k+2}}{\beta_1} - \frac{\beta_{k+1}}{\beta_0} - \frac{1}{\beta_0}\sum_{l=0}^{k-1}\beta_{k-l}\acute{\beta}_l, \qquad (7)$$

with the obvious initial condition $\acute{\beta}_0 = \beta_2/\beta_1 - \beta_1/\beta_0$.

Let $L = 1/\ln(u/\Lambda)$, where Λ is a dimensional parameter, then Eq. (1) becomes $-L^2\frac{\mathrm{d}\alpha}{\mathrm{d}L} = \beta(\alpha)$, or $-\frac{\mathrm{d}L}{L^2} = \frac{\mathrm{d}\alpha}{\beta(\alpha)} = \left[-\frac{1}{\beta_0\alpha^2} + \frac{\beta_1}{\beta_0^2\alpha} + \frac{\beta_1}{\beta_0^2}\acute{\beta}(\alpha)\right]\mathrm{d}\alpha$. Integrating this equation gives $\frac{1}{L} - C' = \frac{1}{\beta_0\alpha} + \frac{\beta_1}{\beta_0^2}\ln\alpha + \frac{\beta_1}{\beta_0^2}\int_0^{\alpha}\acute{\beta}(x)\mathrm{d}x$, or

$$1 - C'L = \frac{L}{\beta_0\alpha} + \frac{\beta_1}{\beta_0^2}L\ln\alpha + \frac{\beta_1 L}{\beta_0^2}\sum_{k=1}^{\infty}\frac{\acute{\beta}_{k-1}}{k}\alpha^k, \qquad (8)$$

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where C' is the constant of integration.

Let $\alpha = \frac{L}{\beta_0} Y(L)$, then

$$\frac{1}{Y} + L^* \ln Y + \sum_{k=1}^{\infty} \grave{\beta}_k L^{*k+1} Y^k = 1 - CL^* - L^* \ln L, \quad (9)$$

where $L^* \equiv (\beta_1/\beta_0^2)L$, $C \equiv (\beta_0^2/\beta_1)C' - \ln\beta_0$, and

$$\grave{\beta}_k \equiv \frac{1}{k}\left(\frac{\beta_0}{\beta_1}\right)^k \acute{\beta}_{k-1}. \quad (10)$$

The graved beta function $\grave{\beta}_k$ can be easily obtained from the expression for the acute beta function $\acute{\beta}_k$ in Eq. (6) or (7), and here are the results:

$$\grave{\beta}_1 = -1 + \dot{\beta}_0\dot{\beta}_2, \quad \grave{\beta}_2 = 1/2 - \dot{\beta}_0\dot{\beta}_2 + (1/2)\dot{\beta}_0^2\dot{\beta}_3, (11)$$

$$\grave{\beta}_3 = -\frac{1}{3} + \dot{\beta}_0\dot{\beta}_2 - \frac{1}{3}\dot{\beta}_0^2(2\dot{\beta}_1\dot{\beta}_3 + \dot{\beta}_2^2) + \frac{1}{3}\dot{\beta}_0^3\dot{\beta}_4, \quad (12)$$

$$\begin{aligned}
\grave{\beta}_{k\geq 4} &= \frac{(-1)^k}{k} + (-1)^{k-1}\dot{\beta}_0\dot{\beta}_2 + \frac{1}{k}\sum_{s=1}^{k-4}\Bigg[(-1)^s\dot{\beta}_0^{k-s-2} \\
&\times \sum_{r=0}^{2}\left(\prod_{p=1}^{s+r}\sum_{l_p=s+r-p+1}^{l_{p-1}-1}\right)B_{l,s}^{(r)}\prod_{q=0}^{s+r-1}\beta_{l_q-l_{q+1}}\Bigg] \\
&+\frac{\dot{\beta}_0^{k-2}}{k}\Bigg[\dot{\beta}_{l_0} + \sum_{l_1=1}^{k-2}(\dot{\beta}_{l_1+1} + \dot{\beta}_2\dot{\beta}_{l_1})\dot{\beta}_{l_0-l_1} \\
&+ \sum_{l_1=2}^{k-2}\sum_{l_2=1}^{l_1-1}\dot{\beta}_{l_0-l_1}\dot{\beta}_{l_1-l_2}\dot{\beta}_{l_2+2}\Bigg] \\
&-\frac{\dot{\beta}_0^{k-1}}{k}\left(\dot{\beta}_k + \sum_{s=0}^{k-2}\dot{\beta}_{l_0-s}\dot{\beta}_{s+2}\right) + \frac{\dot{\beta}_0^k\dot{\beta}_{k+1}}{k}, \quad (13)
\end{aligned}$$

where $l_0 = k-1$, $B_{l,s}^{(0)} = \dot{\beta}_{l_s}$, $B_{l,s}^{(1)} = \dot{\beta}_{l_{s+1}+1} + \dot{\beta}_2\dot{\beta}_{l_{s+1}}$, $B_{l,s}^{(2)} = \dot{\beta}_{l_{s+2}+2}$, and $\dot{\beta}_i = \beta_i/\beta_1$ $(i = 0, 1, 2, \ldots)$.

Now suppose we have a solution of the form

$$Y(L) = \sum_{i=0}^{\infty}\sum_{j=0}^{i} f_{i,j} L^{*i} \ln^j L, \quad (14)$$

then

$$\frac{1}{Y} = \frac{1}{f_{0,0}} + \sum_{i=1}^{\infty}\sum_{j=0}^{i}\left(\sum_{k=1}^{i}\frac{(-1)^k}{f_{0,0}^{k+1}}\underset{1,0}{\textstyle\bigsqcup^k} f_{i,j}\right)L^{*i}\ln^j L, \quad (15)$$

$$L^*\ln Y = \sum_{i=2}^{\infty}\sum_{j=0}^{i-1}\left(\sum_{k=1}^{i-1}\frac{(-1)^{k-1}}{kf_{0,0}^k}\underset{1,0}{\textstyle\bigsqcup^k} f_{i-1,j}\right)L^{*i}\ln^j L, \quad (16)$$

$$\sum_{k=1}^{\infty}\grave{\beta}_k L^{*k+1}Y^k = \sum_{i=2}^{\infty}\sum_{j=0}^{i-2}\left(\sum_{k=2}^{i-j}\grave{\beta}_{k-1}\underset{0,0}{\textstyle\bigsqcup^{l-k}} f_{i-k,j}\right)L^{*i}\ln^j L, \quad (17)$$

where the square cup operator, $\bigsqcup$, has been defined in the appendix. Substituting these expressions into Eq. (9), we can obtain all $f_{i,j}$ by comparing the corresponding coefficients of $u^{*i}\ln^j u$. For $(i,j) = (0,0)$, $(1,0)$, and $(1,1)$, we have $f_{0,0} = 1$, $f_{1,0} = C$, $f_{1,1} = 1$. For $i \geq 2$ and $j = i$, we have $\sum_{k=1}^{i}(-1)^k\bigsqcup_{1,0}^{k}f_{i,i} = 0$, which gives $f_{i,i} = 1$. And for $i \geq 2$ and $j = i-1$, we get

$$\sum_{k=1}^{i}(-1)^k\underset{1,0}{\textstyle\bigsqcup^k} f_{i,i-1} + \sum_{k=1}^{i-1}\frac{(-1)^{k-1}}{k}\underset{1,0}{\textstyle\bigsqcup^k} f_{i-1,i-1} = 0 \quad (18)$$

whose solution is $f_{i,i-1} = iC + \sum_{l=1}^{i-1}(i/l - 1)$.

For $i \geq 2$ and $0 \leq j \leq i-2$, we have

$$\begin{aligned}
f_{i,j} &= \sum_{k=2}^{i}(-1)^k\underset{1,0}{\textstyle\bigsqcup^k} f_{i,j} + \sum_{k=1}^{i-1}\frac{(-1)^{k-1}}{k}\underset{1,0}{\textstyle\bigsqcup^k} f_{i-1,j} \\
&+ \sum_{k=1}^{i-j-1}\grave{\beta}_k\underset{0,0}{\textstyle\bigsqcup^k} f_{i-k-1,j}. \quad (19)
\end{aligned}$$

Please note, there are only terms of $f_{i'<i,j'<j}$ on the right hand side of this equation. Therefore, it is a recursive relation. Here are the solution to order 5:

$$f_{2,0} = C^2 + C + \grave{\beta}_1, \quad (20)$$

$$f_{3,0} = C^3 + \frac{5}{2}C^2 + (3\grave{\beta}_1 + 1)C + \grave{\beta}_1 + \grave{\beta}_2, \quad (21)$$

$$f_{3,1} = 3C^2 + 5C + 3\grave{\beta}_1 + 1, \quad (22)$$

$$\begin{aligned}
f_{4,0} &= C^4 + (13/3)C^3 + (6\grave{\beta}_1 + 9/2)C^2 \\
&+ (1 + 7A_1 + 4\grave{\beta}_2)C + 2\grave{\beta}_1^2 + \Sigma_{i=1}^3\grave{\beta}_i, \quad (23)
\end{aligned}$$

$$\begin{aligned}
f_{4,1} &= 4C^3 + 13C^2 + (12\grave{\beta}_1 + 9)C \\
&+ 7A_1 + 4\grave{\beta}_2 + 1, \quad (24)
\end{aligned}$$

$$f_{4,2} = 6C^2 + 13C + 6\grave{\beta}_1 + 9/2, \quad (25)$$

$$\ldots$$

These correspond to the standard form in Ref. [8] at order 3, and agrees to that in Ref. [9] at order 4, i.e.,

$$\begin{aligned}
\alpha(u) &= \frac{1}{\beta_0 \ln(u/\Lambda)}\Bigg\{1 - \frac{\beta_1 \ln\ln(u/\Lambda)}{\beta_0^2 \ln(u/\Lambda)} \\
&+ \frac{\beta_1^2}{\beta_0^4 \ln^2(u/\Lambda)}\left[\left(\ln\ln\frac{u}{\Lambda} - \frac{1}{2}\right)^2 + \frac{\beta_0\beta_2}{\beta_1^2} - \frac{5}{4}\right] \\
&- \frac{\beta_1^3}{\beta_0^6 \ln^3(u/\Lambda)}\left[\left(\ln\ln\frac{u}{\Lambda} - \frac{5}{6}\right)^3 - \frac{\beta_0^2\beta_3}{2\beta_1^3} + \frac{233}{216} \right. \\
&\left. + \left(3\frac{\beta_0 b_2}{\beta_1^2} - \frac{49}{12}\right)\ln\ln\frac{u}{\Lambda}\right]\Bigg\}. \quad (26)
\end{aligned}$$

To give a general representation for the expansion coefficients $f_{i,j}$, introduce a set of new functions $\bar{\beta}_i$ by the recursive relation

$$\bar{\beta}_i = \sum_{k=1}^{i-1}\left[K\left(\underset{1}{\textstyle\bigsqcup^{k+1}}\bar{\beta}_i - \underset{1}{\textstyle\bigsqcup^k}\bar{\beta}_{i-1}\right) + \grave{\beta}_k\underset{0}{\textstyle\bigsqcup^k}\bar{\beta}_{i-k-1}\right], \quad (27)$$

where $K \equiv (-1)^{k-1}(1+1/k)$. From the initial conditions $\bar{\beta}_0 = 1$ and $\bar{\beta}_1 = C$, one can easily get all $\bar{\beta}_i$ from Eq. (27). For $C = 0$, for example, we have

$$\bar{\beta}_0 = 1, \ \bar{\beta}_1 = 0, \ \bar{\beta}_2 = \dot{\beta}_1, \ \bar{\beta}_3 = \dot{\beta}_1 + \dot{\beta}_2, \quad (28)$$

$$\bar{\beta}_4 = \sum_{i=1}^{3} \dot{\beta}_i + 2\dot{\beta}_1^2, \ \bar{\beta}_5 = \sum_{i=1}^{4}\dot{\beta}_i + \frac{9}{2}\dot{\beta}_1^2 + 5\dot{\beta}_1\dot{\beta}_2, (29)$$

$$\bar{\beta}_6 = \Sigma_{i=1}^{5}\dot{\beta}_i + \frac{15}{2}\dot{\beta}_1^2 + 3\dot{\beta}_2^2 + 11\dot{\beta}_1\dot{\beta}_2 + 5\dot{\beta}_1^3, \quad (30)$$
$$\cdots$$

Please note, even when one sets all $\beta_{i>2}$ to zero, no $\bar{\beta}_{k>2}$ will be zero. This is one of the most important reason for us to know the general relation between $f_{i,j}$ and the beta function.

It is found that $f_{i,j}$ satisfies

$$f_{i,j} = \sum_{k=0}^{i-j} f_{i-j,k} \sum_{l=0}^{j} \frac{(i-l)!}{(i-j)!(j-l)!} \bigsqcup_0^k \Phi_l, \quad (31)$$

where $\bigsqcup_0^k \Phi_l$ are the Taylor coefficients of $\ln^k(1+x)$, i.e., $\ln^k(1+x) = \sum_{l=0}^{\infty}\left(\bigsqcup_0^k \Phi_l\right)x^l = \left(\sum_{l=0}^{\infty}\Phi_l x^l\right)^k = \left(\sum_{l=1}^{\infty}\frac{1}{l}x^l\right)^k$. Accordingly we have $\Phi_0 = 0$, $\Phi_{l\geq 1} = 1/l$, $\bigsqcup_0^0 \Phi_l = \delta_{l,0}$, $\bigsqcup_0^k \Phi_0 = \delta_{k,0}$, $\bigsqcup_0^1 \Phi_l = \Phi_l$, and

$$\bigsqcup_0^{k\geq 2} \Phi_{l\geq 1} = \left(\prod_{s=1}^{k-1}\sum_{p_s=1}^{l-k+s-\Sigma_{q=1}^{s-1}p_q}\right)\frac{1}{l-\Sigma_{q=1}^{k-1}p_q}\prod_{s=1}^{k-1}\frac{1}{p_s}. \quad (32)$$

One can naturally consider to prove Eq. (31) by mathematical induction. We have numerically checked it to order 100. Now we directly used it to give an expression for $f_{i,j}$, i.e.,

$$f_{i,j} = \sum_{k=0}^{i-j} P_{j,k}^{(i)} \bar{\beta}_k, \quad (33)$$

where $P_{j,k}^{(i)}$ can be obtained by repeatedly using Eq. (31). For $k = i-j$ and $k = i-j-1$, it is easy to get

$$P_{j,i-j}^{(i)} = \frac{i!}{j!(i-j)!}, \ P_{j,i-j-1}^{(i)} = \frac{i-j}{(i-j)!}\sum_{l=1}^{j}\frac{(i-l)!}{(j-l)!l}. \quad (34)$$

Generally for $k = i-j-l$ or $l = i-j-k$, careful derivations give

$$P_{j,k}^{(i)} = \mathcal{Q}(i,j,l)\mathcal{Q}(i-j,l,0)$$
$$+ \sum_{r=1}^{l-1}\left\{\left(\prod_{p=1}^{r}\sum_{s_p=1}^{l-1-\Sigma_{q=1}^{p-1}s_q}\right)\left[\mathcal{Q}(i,j,s_1)\right.\right.$$
$$\times \mathcal{Q}\left(i-j-\Sigma_{q=1}^{r-1}s_q, s_r, l-\Sigma_{q=1}^{r}s_q\right)$$
$$\times \mathcal{Q}\left(i-j-\Sigma_{q=1}^{r}s_q, l-\Sigma_{q=1}^{r}s_q, 0\right)$$
$$\left.\left.\times \prod_{p=1}^{r-1}\mathcal{Q}\left(i-j-\Sigma_{q=1}^{p-1}s_q, s_p, s_{p+1}\right)\right]\right\}, \quad (35)$$

where $\mathcal{Q}$ is a function of three non-negative integers and defined by

$$\mathcal{Q}(i,j,k) \equiv \frac{1}{(i-j)!}\sum_{l=0}^{j}\frac{(i-l)!}{(j-l)!}\bigsqcup_0^k \Phi_l. \quad (36)$$

For a given i, one can regard $P^{(i)} = \left[P_{j,k}^{(i)}\right]$ as a matrix of order $i+1$. The specially simple elements are: $P_{i,k\geq i-j}^{(i)} = 0$, $P_{0,k}^{(i)} = \delta_{k,i}$, $P_{1,k}^{(i)} = k+1$, $P_{i,k}^{(i)} = \delta_{k,0}$, $P_{i-1,0}^{(i)} = \sum_{s=1}^{i-1}(i/s - 1)$, $P_{i-1,1}^{(i)} = i$. Here are the $P^{(i)}$ matrix for i from 0 to 4:

$$P^{(0)} = [1], \ P^{(1)} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \ P^{(2)} = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 2 & 0 \\ 1 & 0 & 0 \end{bmatrix},$$

$$P^{(3)} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 2 & 3 & 0 \\ \frac{5}{2} & 3 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \ P^{(4)} = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 2 & 3 & 4 & 0 \\ 9/2 & 7 & 6 & 0 & 0 \\ 13/3 & 4 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix}. (37)$$

In the traditional minimum subtraction scheme ($\overline{\text{MS}}$), the strong coupling $\alpha(u)$ as a function of the renormalization point u is not continuous at the quark masses. Let's derive a matching-invariant coupling by absorbing loop effects into the $\overline{\text{MS}}$ definition and give the corresponding beta function to four-loop level.

Suppose the new coupling α' is connected to the original coupling α by

$$\alpha' = \sum_{i=0}^{\infty} a_i \alpha^{i+1}. \quad (38)$$

Then, using the matching condition $\check{\alpha} = \sum_{j=0}^{\infty}C_j \alpha^{j+1}$ with the matching coefficients [9, 10]

$$C_0 = 1, \ C_1 = 0, \ C_2 = 11/72, \quad (39)$$
$$C_3 = \frac{575263}{124416} - \frac{82043}{27648}\zeta_3 - \frac{2633}{31104}N_{\text{f}}, \ \cdots \quad (40)$$

one has

$$\check{\alpha}' = \sum_{i=0}^{\infty}\left[\sum_{k=0}^{i}\check{a}_k\bigsqcup_0^{k+1}C_{i-k}\right]\alpha^{i+1}, \quad (41)$$

where an overhead check means decreasing N_{f} by one flavor to the corresponding $(N_{\text{f}}-1)$-flavor effective theory. Accordingly, comparing the coefficients of α in the equality $\check{\alpha}' = \alpha'$ yields

$$a_i = \sum_{k=0}^{i}\check{a}_k\bigsqcup_0^{k+1}C_{i-k}. \quad (42)$$

Assume $a_i = \sum_{j=0}^{i}a_{i,j}N_{\text{f}}^j$, then $\check{a}_k = \sum_{j=0}^{k}a_{k,j}(N_{\text{f}}-1)^j$. Substitution into Eq. (42) then gives

$$\sum_{k=0}^{i}\left[a_{i,k}N_{\text{f}}^k - \left(\bigsqcup_0^{k+1}C_{i-k}\right)\sum_{j=0}^{k}a_{k,j}(N_{\text{f}}-1)^j\right] = 0, \quad (43)$$

whose solution is

$$a_0 = a_{0,0}, \quad a_1 = a_{1,0}, \quad a_2 = a_{2,0} + \frac{11}{72}a_{0,0}N_{\rm f}, \quad (44)$$

$$a_3 = a_{3,0} + \left[\left(\frac{7037}{1536} + \frac{82043}{27648}\zeta_3\right)a_{0,0} + \frac{11}{36}a_{1,0}\right]N_{\rm f}$$
$$- \frac{2633}{62208}a_{0,0}N_{\rm f}^2, \quad \cdots \quad (45)$$

To definitely fix the new coupling, one needs to choose $a_{i,0}$. The simplest choice would be $a_{i,0} = \delta_{i,0}$. With this convention, one has

$$a_0 = 1, \quad a_1 = 0, \quad a_2 = (11/72)N_{\rm f}, \quad (46)$$

$$a_3 = a_{3,1}N_{\rm f} - \frac{2633}{62208}N_{\rm f}^2, \quad \cdots \quad (47)$$

where $a_{3,1} = 7037/1536 + 82043\zeta_3/27648 \approx 8.148377983$. Then the new matching-invariant coupling is

$$\alpha' = \alpha + \frac{11}{72}N_{\rm f}\alpha^3 + \left(a_{3,1} - \frac{2633}{62208}N_{\rm f}\right)N_{\rm f}\alpha^4 + \cdots \quad (48)$$

The renormalization equation for α' is

$$u\frac{{\rm d}\alpha'}{{\rm d}u} = -\sum_{i=0}^{\infty}\beta_i'\alpha'^{i+2}. \quad (49)$$

The primed beta function β_i' can be obtained as such. Operating with $u\frac{\rm d}{{\rm d}u}$ on both sides of Eq. (38), applying Eqs. (49) and (1), and then comparing coefficients will give $\sum_{k=0}^{i}\left[\beta_k'\bigsqcup_0^{k+2}a_{i-k} - (k+1)a_k\beta_{i-k}\right] = 0$, namely, β_i' are given by the recursive relation

$$\beta_i' = \sum_{k=0}^{i}(k+1)a_k\beta_{i-k} - \sum_{k=0}^{i-1}\beta_k'\bigsqcup_0^{k+1}a_{i-k}. \quad (50)$$

On application of Eqs. (46) and (47), one immediately has the following explicit expressions for the new beta function:

$$\beta_0' = \beta_0 = 11/2 - N_{\rm f}/3, \quad (51)$$
$$\beta_1' = \beta_1 = 51/4 - (19/12)N_{\rm f}, \quad (52)$$
$$\beta_2' = \beta_2 + a_2\beta_0 - a_1(\beta_1 + a_1\beta_0)$$
$$= \frac{2857}{64} - \frac{4549}{576}N_{\rm f} + \frac{79}{576}N_{\rm f}^2, \quad (53)$$
$$\beta_3' = \beta_3 + 2a_3\beta_0 - 2a_1\beta_2 + a_1^2\beta_1 + 4a_1^3\beta_0 - 6a_1a_2\beta_0$$
$$= \beta_3^{(0)} + \beta_3^{(1)}N_{\rm f} + \beta_3^{(2)}N_{\rm f}^2 + \frac{10085}{186624}N_{\rm f}^3, \quad (54)$$
$$\cdots$$

with $\beta_3^{(0)} = 149753/768 + (891/32)\zeta_3 \approx 228.4606573$, $\beta_3^{(1)} = 2118091/82944 + (2603291/55296)\zeta_3 \approx 82.12826576$, $\beta_3^{(2)} = -4027/1296 - (194353/82944)\zeta_3 \approx -5.923892810$.

It should be mentioned that a different expression for β_2' was previously given in Ref. [11]. The difference is caused by the fact that a wrong value for C_2 was quoted there [12].

As an application of the general relation between $f_{i,j}$ and the beta function, one can develop another expansion which converges much faster. For this one can observe, more carefully, the standard expansion

$$\alpha = \sum_{i=0}^{\infty}\frac{\beta_0}{\beta_1}L^{*i+1}\sum_{j=0}^{i}f_{i,j}\ln^j L \equiv \sum_{i=0}^{\infty}J_i. \quad (55)$$

Representing the terms in this expansion with the corresponding coefficients $f_{i,j}$, all the terms can be arranged in a matrix as

$$[f_{i,j}] = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ f_{1,0} & 1 & 0 & 0 & 0 \\ f_{2,0} & f_{2,1} & 1 & 0 & 0 & \vdots \\ f_{3,0} & f_{3,1} & f_{3,2} & 1 & 0 \\ f_{4,0} & f_{4,1} & f_{4,2} & f_{4,3} & 1 \\ & & \cdots & & \end{bmatrix}. \quad (56)$$

The standard expansion corresponds to summing the terms row by row. When one takes the expansion to a finite order, i.e., replacing the ∞ in Eq. (55) with a positive integer N, as has been done in the usual way, then all the terms like $f_{j,j}$ $(N < j < \infty)$ on the diagonal and $f_{j+1,j}$ on the next to diagonal are missed, although these terms are all known and have nothing to do with beta functions. Generally, the terms $f_{j+k,j}$ for $0 < j < \infty$ on the kth next to diagonal involves only $\beta_{0 \le l \le k-2}$. But all the terms $f_{j+k,j}$ with $j > N$ are lost, though no such terms are zero even when one sets all $\beta_{i>2}$ to zero.

To include the contribution from the terms just mentioned, we can consider to sum over diagonals, which can be achieved by taking $i = j + k$ in Eq. (55), i.e.,

$$\alpha = \frac{\beta_0}{\beta_1}\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}f_{j+k,j}(L^*\ln L)^j L^{*k+1} \equiv \sum_{k=0}^{\infty}I_k, \quad (57)$$

where the expressions for $f_{j+k,j}$ can be obtained from Eq. (33):

$$f_{j,j} = 1, \quad f_{j+1,j} = \sum_{l=1}^{j}\left(\frac{j+1}{l} - 1\right) + (j+1)C, \quad (58)$$

$$f_{j+2,j} = \frac{\bar{\beta}_2}{2}(j+1)(j+2) + \left(C + \frac{1}{2}\right)\sum_{s=0}^{j-1}\frac{(s+1)(s+2)}{j-s}$$
$$+ \frac{1}{2}\sum_{s=0}^{j-2}\sum_{r=1}^{j-s-1}\frac{(s+1)(s+2)}{r(j-s-r)}, \quad \cdots \quad (59)$$

From these expressions, we can give compact form to I_k:

$$I_0 = \frac{L}{\beta_0}\sum_{j=0}^{\infty}(L^*\ln L)^j = \frac{L/\beta_0}{1 - L^*\ln L} \equiv \beta_0 X, \quad (60)$$

$$I_1 = \beta_0\beta_1 X^2[C - \ln x], \quad (61)$$
$$I_2 = \beta_0\beta_1^2 X^3\left[f_{2,0} - f_{2,1}\ln x + \ln^2 x\right], \quad (62)$$

where $x \equiv 1 + (\beta_1/\beta_0^2) \ln \ln(u/\Lambda)/\ln(u/\Lambda)$, and $X \equiv L^*/(\beta_1 x) = 1/[\beta_0^2 \ln(u/\Lambda) + \beta_1 \ln \ln(u/\Lambda)]$.
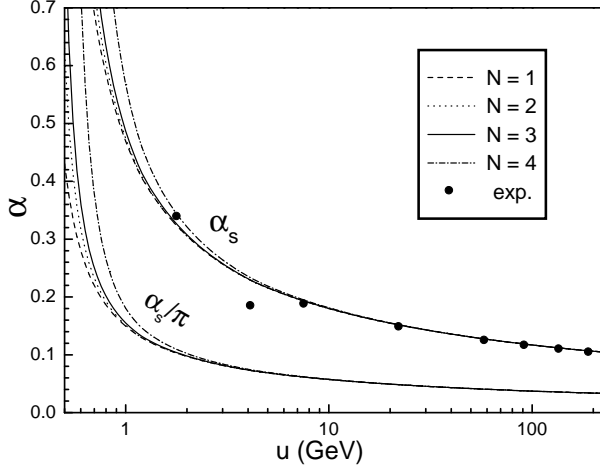

FIG. 1: The QCD coupling as functions of the t'Hooft unit of mass. The dot, dash, solid, and dot-dash lines are, respectively, for the order N from 1 to 4 with the scale Λ indicated in Tab. 1. The full dots are the experimental data of, in increasing order of Λ, τ width, Υ decay, deep inelastic scattering, e^+e^- event shapes at 22 GeV from the JADE data, shapes at TRISTAN at 58 GeV, Z width, and e^+e^- event shapes at 135 and 189 GeV.
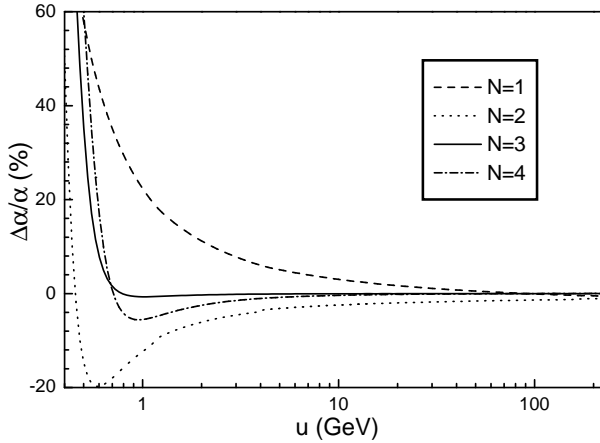

FIG. 2: The relative difference between the new expansion in Eq. (63) and the conventional expansion in Eq. (55).

In Eq. (57), there are an infinite number of logarithmic terms like $\ln^j x$ which are included in I_k, even when one takes the expansion to a finite order, say $\alpha = \sum_{k=0}^{N} I_k$. The first several I_ks have been worked out to a closed form in Eqs. (60)–(62). The procedure is, to some extent, similar to that in Ref. [13] for the matching function. Here we can, in fact, give the closed form for I_k to arbitrary order:

$$\alpha = \sum_{k=0}^{\infty} \beta_0 \beta_1^k X^{k+1} \sum_{l=0}^{k} (-1)^l f_{k,l} \ln^l x. \qquad (63)$$

In Eqs. (63) and (55), there are two arbitrary constants: Λ and C. Because the renormalization group equation (49) or (1) is of the first order, only one of them is independent. So we can arbitrarily take one of them, while the other is determined by giving an initial condition. It nearly becomes standard, nowadays, to take $C = 0$ [14], which makes expressions somewhat simpler, and $\alpha(m_Z) = 0.1187/\pi$, where $M_Z = 91.1876$ GeV is the mass of Z bosons. Setting $C = 0$ requires distinct Λ for different effective flavor regimes, and we use Λ_6, Λ_5, Λ_4, and Λ_3 for $u > m_t$, $m_b < u < m_t$, $m_c < u < m_b$, and $m_s < u < m_c$, respectively, where the relevant quark masses are taken, in the present calculations, to be $m_t = 175$ GeV, $m_b = 4.2$ GeV, $m_c = 1.2$ GeV, and $m_s = 100$ MeV.

In Fig. 1, the coupling is shown as a function of the renormalization point, calculated from Eq. (63) with the infinity replaced by N, and the order N from 1 to 4. The same calculation has also been performed from the conventional expansion in Eq. (55). The relative difference between the results from Eq. (63) and Eq. (55) is shown in Fig. 2. It can be seen that, with decreasing u, the difference becomes more and more significant.

TABLE I: QCD renormalization group scale parameter Λ for the order from 1 to 4. For each Λ_i, the left column is for the new expansion in Eq. (63) and the right column is for the conventional expansion in Eq. (55).

Λ (MeV)	Λ_6		Λ_5		Λ_4		Λ_3	
$N = 1$	88	45	208	91	286	124	325	147
$N = 2$	91	95	217	235	303	335	350	377
$N = 3$	90	90	214	212	298	294	340	334
$N = 4$	88	86	209	207	295	291	344	342

To compare the convergence speed of Eqs. (63) and (55), all the Λ_i ($i = 3$–6) are listed in Tab. I. There are two columns corresponding to each Λ_i, the left column is for Eq. (63) while the right column is for Eq. (55). It is obvious that the new expansion (63) converges much faster than the original expansion (55). Even at the leading-order ($N = 1$), the corresponding Λ_i for Eq. (63) has nearly approached to its value at order 4. So in practical applications, it should be very accurate to calculate the coupling simply by

$$\alpha = \frac{\beta_0}{\beta_0^2 \ln(u/\Lambda) + \beta_1 \ln \ln(u/\Lambda)}. \qquad (64)$$

In summary, the general relation between the standard expansion coefficients and the beta function is carefully derived. A matching-invariant coupling is given with the corresponding beta function to four-loop level. A new expansion for the coupling is then deduced, which is in principle more accurate than the conventional expansion due to the inclusion of an infinite number of logarithmic terms in a closed form.

APPENDIX A: SQUARE CUP OPERATOR

The square cup operator, $\bigsqcup_m^k$, is defined so that it meets

$$\left(\sum_{i=m}^{\infty} a_i x^i\right)^k = \sum_{i=0}^{\infty} \left(\bigsqcup_m^k a_i\right) x^i. \qquad (A1)$$

Obviously one has $\bigsqcup_m^0 a_i = \delta_{i,0}$, $\bigsqcup_m^1 a_{i<m} = 0$, $\bigsqcup_m^1 a_{i\geq m} = a_i$. And for $k \geq 2$, it is also not difficult to give a general explicit expression

$$\bigsqcup_m^k a_i = \left(\prod_{s=1}^{k-1} \sum_{p_s=m}^{i-(k-s)m-\varsigma_s^p}\right) a_{i-\varsigma_k^p} \prod_{r=1}^{k-1} a_{p_r} \qquad (A2)$$

where

$$\varsigma_s^p \equiv \begin{cases} \sum_{t=1}^{s-1} p_t & \text{if } s > 1 \\ 0 & \text{otherwise} \end{cases}. \qquad (A3)$$

The meaning of ς_k^p is similar to this. Here are several special simple cases:

$$\bigsqcup_m^k a_0 = \delta_{k,0}, \quad \bigsqcup_m^k a_{i\leq km} = 0, \quad \bigsqcup_m^k a_{km} = a_m^k, \qquad (A4)$$

The two-dimensional extension of the square cup operator, $\bigsqcup_{m,n}^k$, is defined by

$$\left(\sum_{i=m}^{\infty} \sum_{j=n}^{i} f_{i,j} x^i y^j\right)^k = \sum_{i=0}^{\infty} \sum_{j=0}^{i} \left(\bigsqcup_{m,n}^k f_{i,j}\right) x^i y^j. \quad (A5)$$

Similarly, one has $\bigsqcup_{m,n}^0 f_{i,j} = \delta_{i,0}\delta_{j,0}$, $\bigsqcup_{m,n}^1 f_{i<m,j<n} = 0$, $\bigsqcup_{m,n}^1 f_{i\geq m,j\geq n} = f_{i,j}$. And for $k \geq 2$, we have

$$\bigsqcup_{m,n}^k f_{i,j} = \left(\prod_{s=1}^{k-1} \sum_{p_s=m}^{i-(k-s)m-\varsigma_s^p} \sum_{q_s=\sigma}^{p_s^*}\right) f_{i-\varsigma_k^p, j-\varsigma_k^q} \prod_{r=1}^{k-1} f_{p_r,q_r} \qquad (A6)$$

where

$$p_s^* \equiv \min\left[p_s, j - (k-s)n - \varsigma_s^q\right], \qquad (A7)$$

$$\sigma \equiv \max\left(n, \sum_{t=1}^{s} p_t - \varsigma_s^q - i + j\right). \qquad (A8)$$

Here are special examples:

$$\bigsqcup_{m,n}^k f_{0,0} = \delta_{k,0}, \quad \bigsqcup_{m,n}^k f_{i<km,j<kn} = 0, \quad \bigsqcup_{m,n}^k f_{km,kn} = f_{m,n}^k. \qquad (A9)$$

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[1] G.X. Peng, Europhys. Lett. **72** (2005) 69; Nucl. Phys. A **747** (2005) 75.

[2] E.S. Fraga and P. Romatschke, Phys. Rev. D **71** (2005) 105014; E.S. Fraga, R.D. Pisarski, and J. Schaffner-Bielich, Phys. Rev. D **63** (2001) R121702.

[3] D.J. Gross and F. Wilczek, Phys. Rev. Lett. **30** (1973) 1343; Phys. Rev. D **8** (1973) 3633; ibid., **9** (1974) 980; H.D. Politzer, Phys. Rev. Lett. **30** (1973) 1346.

[4] W.E. Caswell, Phys. Rev. Lett. **33** (1974) 244; D.R.T. Jones, Nucl. Phys. B **75** (1974) 531; E.S. Egorian, O.V. Tarasov, Theor. Mat. Fiz. **41** (1979) 26.

[5] O.V. Tarasov, A.A. Vladimirov, A.Yu. Zharkov, Phys. Lett. B **93** (1980) 429; S.A. Larin, J.A.M. Vermaseren, Phys. Lett. B **303** (1993) 334.

[6] S.A. Larin, T. van Ritbergen, and S.A.M. Vermaseren, Phys. Lett. B **400** (1997) 379.

[7] G. t'Hooft, Nucl. Phys. B **61** (1973) 455; W.A. Bardeen,

A.J. Buras, D.W. Duke, and T. Muta, Phys. Rev. D **18** (1978) 3998.

[8] S. Eidelman *et al.* [Particle Data Group Collabration], Phys. Lett. B **592** (2004) 1.

[9] K.G. Chetyrkin, B.A. Kniehl, and M. Steinhauser, Phys. Rev. Lett. **79** (1997) 2184.

[10] G. Rodrigo and A. Santamaria, Phys. Lett. B **313** (1993) 441.

[11] W.J. Marciano, Phys. Rev. D **29** (1984) 580.

[12] W. Bernreuther and W. Wetzel, Nucl. Phys. B **197** (1982) 228; Erratum-ibid. B **513** (1998) 758.

[13] S.D. Bass, R.J. Crewther, F.M. Steffens, and A.W. Thomas, Phys. Rev. D **68** (2003) 096005.

[14] W.A. Bardeen, A. Buras, D. Duke, and T. Muta, Phys. Rev. D **18** (1978) 3998; A. Burus, Rev. Mod. Phys. **52** (1980) 199.